In The Claims

Please replace Claim 22 with the following:

B4

22. (Amended) A method of determining a shape space of a set of molecules, comprising:

choosing an initial set of N molecules wherein N is less than a total number of molecules in the set of molecules and N is at least 2, and a property of the set of molecules;

calculating a distance matrix D wherein each element D_{ij} is a minimal metric distance between said property of a molecule i and said property of a molecule j and wherein said molecule i and said molecule j are in said initial set of molecules;

constructing a metric matrix G from D according to a distance geometry technique;

diagonalizing G, thereby obtaining eigenvalues of G, and obtaining a set of positions in N-1-dimensional space that reproduce the distances in said matrix D to within a tolerance T, wherein each position of said set of positions has N-1 coordinates associated with it;

determining which of the N-1 coordinates that represent positions in shape space of each of the N molecules can be eliminated for every molecule such that a remaining number, M, of the N-1 coordinates still enables said distance matrix to be reproduced to within said tolerance, T; and

defining the shape space to be an M dimensional subspace occupied by the N molecules.
